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- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Identifying the charge and magnetic structures in the bilayer ferrates	**Experiment number**: 28-01-847
Beamline: BM28	**Date of experiment**: from: 18/02/2009 to: 24/02/2009	**Date of report**: 08/11/2009
Shifts: 18	**Local contact(s)**: BOUCHENOIRE, Laurence	*Received at ESRF:*

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Report:

Charge disproportionation and ordering has been the subject of a substantial number of studies in condensed matted physics, and represents a key concept in helping us understand a range of interesting phenomena. A variety of transition metal oxides display a degree of charge disproportionation at equivalent crystallographic sites, such as magnetoresistive manganites [1] and superconducting stripes in cuprates [2]; with the stripes' dynamic fluctuations being suggested as a mechanism for high temperature superconductivity [3].

The original brief of this experiment was to study the charge order in the bilayer ferrates. These systems are of interest, as the highly 2-dimensional nature of the crystal structure allows us to study the driving force behind charge order in a single plane. The ferrates are the model system to study the charge interaction as it appears as though there are no Jahn-Teller distortions present in this series, suggesting no orbital order is present, greatly simplifying the problem. However, at the time of the experiment, single crystals of sufficient quality were not available. With this being the case we instead studied alternate perovskite ferrates: the pseudocubic $Nd_xSr_{1-x}FeO_3$ and $CaFeO_3$.

Even after numerous studies $CaFeO_3$ remains a system that is not fully understood. Above 290 K the system possesses Fe sites with a valence of 4+; however, upon cooling the system reportedly charge disproportionates, to Fe 3+ and unusually high 5+ ions (4,5,6). There is also uncertainty surrounding the low temperature magnetic order of $CaFeO_3$. In this material neutron powder diffraction has determined the existence of long range magnetic order below 115 K, although Reitveld refinement of this data provides two possibilities; either a screw spiral structure in the [101]

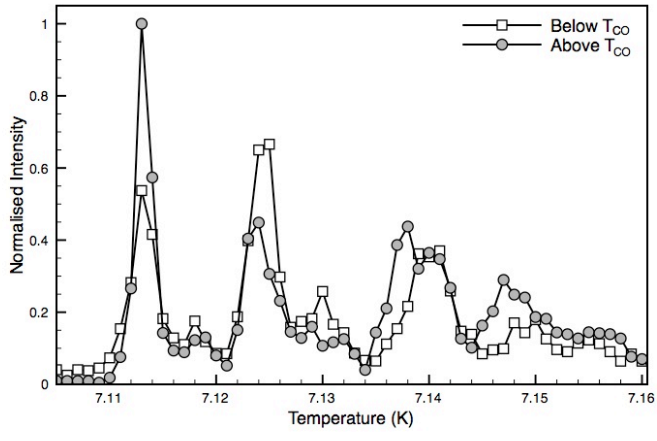

Fig 1. Energy dependence of the (1 0 2) ATS reflection in $CaFeO_3$, above and below the charge ordering transition.

direction[6,7], or a sinusoidal amplitude modulated structure with the Fe ordered along [010] [ref. 6]. In order to address the question of the amount of charge disproportionation we attempted to perform energy scans of ATS reflections in both phases, to be simulated using the FDMNES code as previously performed on Fe_3O_4 [8.9]. However, we were plagued by multiple scattering, and attempts to combat this met with limited success. As can be seen in Fig 1, the data obtained above and below T_{CO} is not qualitatively different within the region of uncertainty produced by the multiple scattering contamination.

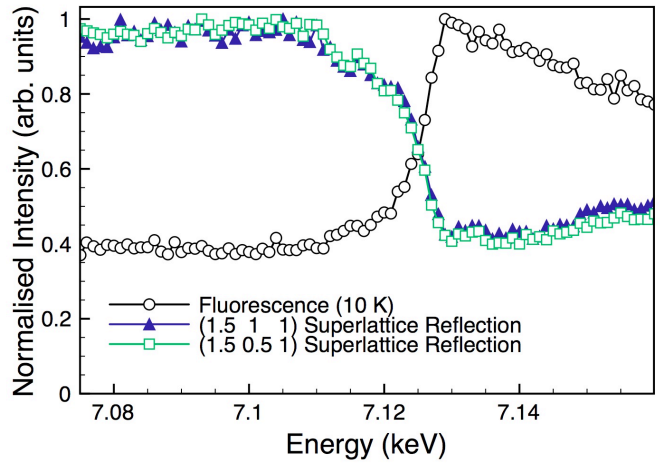

Fig 2. Energy dependence of charge order reflections in $Nd_{0.5}Sr_{0.5}FeO_3$.

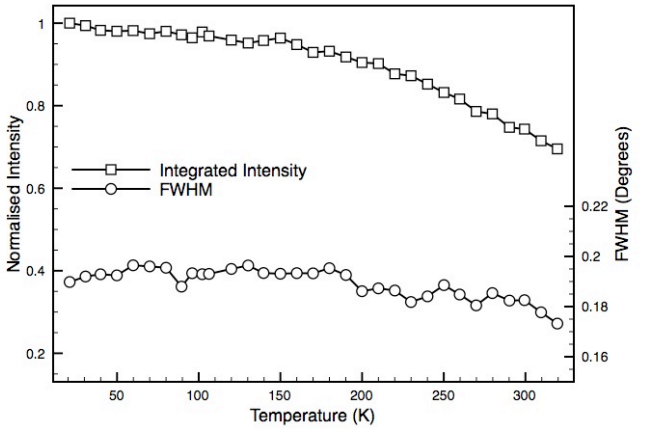

Fig 3. Temperature dependence of the (1.5 0.5 1) charge order reflection in $Nd_{0.5}Sr_{0.5}FeO_3$.

The rest of the experiment was devoted to performing the first diffraction experiment on $Nd_{0.5}Sr_{0.5}FeO_3$. Our study of the charge order reflections in $Nd_{0.5}Sr_{0.5}FeO_3$ revealed that many of the charge order reflections show no resonant effect, Fig 2. This may be because the crystallographic strain wave associated with the charge order masks the resonant behaviour, or because large resonances only appear at certain reflections. In the related manganite compound, $Nd_{0.5}Sr_{0.5}MnO_3$, both resonating and non-resonating charge order reflections have been reported, as well as orbital order reflections with large resonant effects [10,11]. However, it appears both charge and orbital resonant reflections show the same azimuthal dependence, which may indicate they have the same origin; *i.e.* they are structural ATS reflections. By locating the same reflections in $Nd_{0.5}Sr_{0.5}FeO_3$ in a devoted study we hope to address two key questions: what are the origins of these reflections (charge/orbital/structural ATS); and what is the magnitude of the charge disproportionation in the lower doped ferrates. We also revealed that this ferrate possess a significantly higher ordering temperature than any other perovskite ferrate yet studied. At the time of the experiment, the time constraints of changing cryostat meant that we were unable to heat above 320 K, Fig 3. However, by 320 K the intensity had only diminished by ~20%, with little change in the width: suggesting a transition temperature in the region of 600 K. It is our intention to determine the full temperature dependence of the charge order in a follow up study.

References

[1] Mori S, Chen C H and Cheong S –W, *Nature* **392** 473-476 (1998) [2] Tranquada J M *et al*., *Nature* **375** 561-563 (1995) [3] Salkola M I, Emery V J, and Kivelson S A, *Phys. Rev. Lett*. **77** 155-158 (1996) [4] M. Takano *et al*., Mater. Res. Bull. **12**, 923 (1977) [5] S. Morimoto *et al.* Physica B 237-238 (1997) 66 67 [6] P.M. Woodward,*et al*., *Phys. Rev. B* **62** 844 (2000). [7] S. Kawasaki *et al*., *J. Phys. Soc. Jap.* **67** 1529 (1998). [8] E. Nazarenko *et al. Phys. Rev. Lett.* 97, 056403 (2006) [9] S. R. Bland *et al. Journal of Physics: Condensed Matter* **21**: 485601. [10] M. E. Ghazi, PhD Thesis, Durham University (2002). [11] K. Nakamura *et al.,* Phys. Rev. B, **60**, 2425 (1999).